

COORDINATION SEQUENCES AND CRITICAL POINTS

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Coordination sequences of periodic and quasiperiodic graphs are analysed. These count the number of points that can be reached from a given point of the graph by a number of steps along its bonds, thus generalising the familiar coordination number which is just the first member of this series. A possible application to the theory of critical phenomena in lattice models is outlined.

1 Introduction

The locations of critical points of lattice models (such as Ising models, percolation problems or self-avoiding walks) depend on the topological structure of the underlying graph, in particular on the dimension and on the (mean) coordination number.^{1–5} However, this can only be a first approximation, and more detailed information on the graph is required for a better understanding of the precise location of critical points. For this purpose, quasiperiodic graphs prove helpful because they provide different cases with the same mean coordination number and also a check of the “universality” of this approach.

Below, we display first results on the combinatorial issue to calculate the coordination sequences, and on general tendencies visible. To this end, we summarise the results for root graphs^{6,7} and present the averaged coordination numbers for the rhombic Penrose and for the Ammann-Beenker tiling.

2 Coordination sequences

A natural family of periodic graphs is given by the so-called root lattices and their relatives, the root graphs,⁷ encoded by the Dynkin diagrams of A_n , B_n ($n \geq 2$), C_n ($n \geq 3$), D_n ($n \geq 4$), G_2 , F_4 , E_6 , E_7 , and E_8 . In all these cases, the coordination sequences $s(k)$, where $s(k)$ is the number of k -th neighbours and $s(0) := 1$, can be calculated completely and encapsulated in an ordinary

Table 1: First coordination numbers of the Penrose tiling [$\tau = (1 + \sqrt{5})/2$].

| k | $s(k)$ | num. value | k | $s(k)$ | num. value |
|-----|------------------|------------|-----|--------------------|------------|
| 1 | 4 | 4.000 000 | 6 | $980 - 588\tau$ | 28.596 015 |
| 2 | $58 - 30\tau$ | 9.458 980 | 7 | $-1614 + 1018\tau$ | 33.158 601 |
| 3 | $-128 + 88\tau$ | 14.386 991 | 8 | $2688 - 1638\tau$ | 37.660 326 |
| 4 | $288 - 166\tau$ | 19.406 358 | 9 | $-3840 + 2400\tau$ | 43.281 573 |
| 5 | $-374 + 246\tau$ | 24.036 361 | 10 | $4246 - 2594\tau$ | 48.819 833 |

generating function of the form

$$S(x) = \sum_{k=0}^{\infty} s(k) x^k = \frac{P(x)}{(1-x)^n} \quad (1)$$

where n is the dimension of the lattice (resp. the graph) and $P(x)$ is an integral polynomial of degree n . For the (hyper-)cubic lattice \mathbb{Z}^n , this polynomial is simply $P_n(x) = (1+x)^n$. For the other cases, the result is

$$\begin{aligned} P_{A_n}(x) &= \sum_{k=0}^n \binom{n}{k}^2 x^k, & P_{B_n}(x) &= \sum_{k=0}^n \left[\binom{2n+1}{2k} - 2k \binom{n}{k} \right] x^k, \\ P_{C_n}(x) &= \sum_{k=0}^n \binom{2n}{2k} x^k, & P_{D_n}(x) &= \sum_{k=0}^n \left[\binom{2n}{2k} - \frac{2k(n-k)}{n-1} \binom{n}{k} \right] x^k, \end{aligned} \quad (2)$$

the expressions for the exceptional cases can be found in Refs. 6 and 7. Many other cases can be calculated, in particular periodic graphs with more complicated fundamental domains, where an averaging procedure over the possible starting points is necessary. Details on this will be given elsewhere.

In view of the applications, one is interested in a variety of graphs that share the same mean coordination number, but have different (averaged) higher coordination numbers. Such examples are provided by planar rhombic tilings with N -fold rotational symmetry. As they are solely built from rhombi, the average coordination number is always exactly four, but the second (and higher) numbers may vary. To expand on this, we present the coordination numbers for two examples, the rhombic Penrose and the Ammann-Beenker tiling (also known as the standard octagonal tiling). The values for the Penrose tiling given in Table 1 were obtained by an exact window algorithm, whereas the results for the Ammann-Beenker case in Table 2 are conjectures based on the averaged coordination numbers of a periodic approximant with 275807 vertices.

Table 2: First coordination numbers of the octagonal tiling ($\lambda = 1 + \sqrt{2}$).

| k | $s(k)$ | num. value | k | $s(k)$ | num. value |
|-----|----------------------|------------|-----|-----------------------|------------|
| 1 | 4 | 4.000 000 | 11 | $360 - 128\lambda$ | 50.980 664 |
| 2 | $48 - 16\lambda$ | 9.372 583 | 12 | $828 - 320\lambda$ | 55.451 660 |
| 3 | $-24 + 16\lambda$ | 14.627 417 | 13 | $-508 + 236\lambda$ | 61.754 401 |
| 4 | $28 - 4\lambda$ | 18.343 146 | 14 | $-996 + 440\lambda$ | 66.253 967 |
| 5 | $52 - 12\lambda$ | 23.029 437 | 15 | $2580 - 1040\lambda$ | 69.217 895 |
| 6 | $48 - 8\lambda$ | 28.686 282 | 16 | $1620 - 640\lambda$ | 74.903 320 |
| 7 | $-324 + 148\lambda$ | 33.303 607 | 17 | $-5288 + 2224\lambda$ | 81.210 963 |
| 8 | $732 - 288\lambda$ | 36.706 494 | 18 | $2372 - 948\lambda$ | 83.325 543 |
| 9 | $380 - 140\lambda$ | 42.010 101 | 19 | $1324 - 512\lambda$ | 87.922 656 |
| 10 | $-1140 + 492\lambda$ | 47.793 073 | 20 | $1196 - 456\lambda$ | 95.118 616 |

3 Critical points

So far, only rudimentary results exist. Critical points of periodic systems have been investigated in some detail, but the results are not fully convincing, and they are still rather incomplete. Furthermore, most results concern hypercubic lattices and hence graphs with different dimensions and coordination numbers, which obscures the dependence on higher order coordination numbers.

For the problem of self-avoiding walks, there exist results also on a variety of quasiperiodic tilings,² and their analysis supports our claim that higher order coordination numbers move the location. In particular, it is clearly seen that the critical point increases with growing second coordination number, while the critical exponents seem to be universal, as expected. However, in order to arrive at a conclusive statement, more, and in particular more precise, data on graphs with coinciding dimension and mean coordination number are needed.

4 Outlook

It is an open question whether one can find explicit expressions for the generating functions $S(x)$ for quasiperiodic graphs. Clearly, these will not have the form of Eq. (1) — an analysis of the generating functions of periodic approximants shows that the polynomial degrees of numerator and denominator grow with the size of the approximant. Still, the coordination sequences show quite a regular behaviour, compare Fig. 1, also when compared to slightly more complicated periodic graphs as, for instance, the Kagomé and the diced lattice. The latter show some similarity to the (dual) Penrose tiling with regard to high-temperature expansions.⁸ Their mean coordination numbers $s(k)$ grow linearly with k , but with two different slopes for even and for odd values of k .

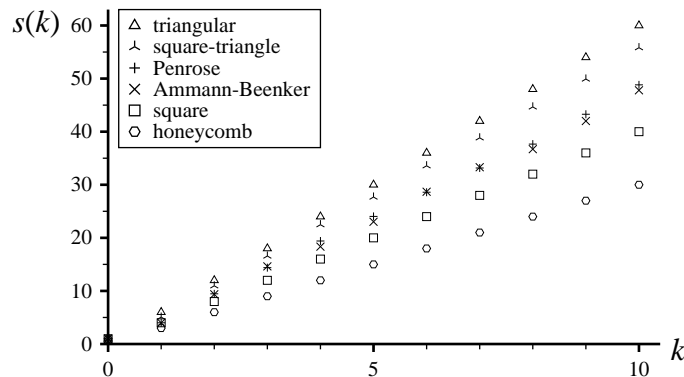


Figure 1: Coordination sequences of some periodic and quasiperiodic graphs.

Ideally, one would hope for a kind of integral transform from the generating function of the combinatorial problem to the partition sum of the corresponding model of statistical mechanics. Such a transformation, however, cannot exist in general since these models are usually not solvable, so their partition sums have an analytic behaviour incompatible with that of our generating functions.

Therefore, one can only expect an empirical formula for the correction to the location of critical points due to higher order coordination numbers. To get a better understanding of this, we intend to analyse the critical structure of various models and on a variety of graphs in the near future.

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